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Mixing in a Semicontinuous Flow System

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ABSTRACT

This paper describes a methodology for measuring and characterizing the degree of mixing in a semicontinuous flow system. The study is restricted to near-instantaneous injection of constant volume feed pulses at regular intervals but the method can be applied to the broader problem of irregular pulses of unequal volume with a finite injection period. Mathematical models for the limiting cases of zero-mixing and complete-mixing are developed and a method of characterizing partial degrees of mixing is described. The development of a model to describe partial mixing in a given system is shown to involve the estimation of parameters in a transfer function using measurements of input-output concentration of a suitable tracer. The transfer function can then be decomposed into elements which can be interpreted as representing sub-regions of either complete or zero mixing in the overall system. A case study is provided to demonstrate the application of the proposed method.

INTRODUCTION

The performance of a flow system involving chemical reaction is determined by the combined effect of the degree of mixing inherent in the flow structure, and the kinetics of the reaction. The theory of the case of continuous steady flow systems is well established and is based on the pioneering work carried out by Danckwerts (1953) on residence-time distributions. Since then a vast body of knowledge has accumulated relating to the measurement and interpretation of residence-time distribution, and its application to the design of reacting flow systems. Levenspiel (1984) is a useful recent source.

In many instances of practical interest the flow is neither continuous nor steady, and for these the theory is not so well established. The proposed paper deals with the case of a semicontinuous flow system in which the feed is injected in discrete amounts at regular intervals of time, thereby displacing equal amounts of effluent fluid. The basis of this work arose from the author's interest in laboratory simulations of waste stabilization ponds in which the quality of a domestic waste-water is improved by the conversion of organic matter into biomass and other metabolites. The available experimental simulations involved semi-continuous operation as described above and their interpretation required an understanding of the mixing inherent in the feed injection process.

The paper explains the basis of residence-time models developed to describe the mixing in a semicontinuous flow system covering the range of complete mixing to zero mixing of the injected fluid. A case study is then used to illustrate the measurement and interpretation of the mixing in an actual semicontinuous flow system. The paper concludes with an overview of the wider implications of the work.

THEORETICAL BACKGROUND

Description of the semicontinuous flow system

Consider the flow system schematically represented in Figure 1. The actual system may be open, as in a pond or lagoon, or closed, as in a conventional chemical reactor. Material is fed to the system as a regular sequence of constant volume pulses and the injection process is assumed to be near-instantaneous in the mathematical model developed in this paper. (The broader problem of irregular pulses of unequal volume with a finite injection period is currently under investigation as an extension of the more restricted system described here). In practice the feed usually contains a reactant material which undergoes chemical transformation inside the flow system, as for example in a waste-stabilization pond where dissolved organic matter undergoes aerobic biodegradation. The extent of reaction is determined by the combined effect of the kinetics of reaction and the degree of mixing present in the reaction zone. The injection process similarly causes a corresponding sequence of constant volume effluent pulses to be discharged from the system so that the volume of the reaction zone remains constant at all times. The problem examined in this paper is the measurement and characterization of the degree of mixing in such a system. This information is an essential ingredient in the design or performance evaluation of a semicontinuous reacting system operated in close conformity with the defined conditions.

Methodology

Suppose that a suitable tracer is dissolved in one of the pulses and let the time of its injection be designated as the origin for time measurement. All previous pulses and all subsequent pulses are free from tracer. The sequence of effluent pulses is then monitored for tracer content and the results expressed as a fraction of the original tracer injected. In this way the residence-time history of injected material can be ascertained, as follows:-

let v be the volume of a pulse

c_i be the tracer concentration in the injected pulse

c_k be the tracer concentration in the k-th effluent pulse

T be the interval between pulses

f_k be the fraction of inlet pulse with residence-time K.T

Then $$f_k = c_k/c_i \qquad (1)$$

This data, if required, can then be converted to a cumulative residence-time distribution by simple summation.

Interpretation of residence-time data

Following the practice used for continuous flow systems it is useful to consider the limiting cases of complete-mixing and zero-mixing, and then use them to formulate descriptions for intermediate mixing.

(a) Complete-mixing. If the entering pulse of fluid first displaces an equal volume pulse of the existing fluid in the system and then completely mixes with the residual fluid in the system, this process can be described as follows:-

$$v.\ u_{k-1} + (V - v).\ c_{k-1} = V.\ c_k \quad (2a)$$

where v is pulse volume
V is system volume
u is tracer concentration, entering pulse
c is tracer concentration, displaced pulse
k is the k the pulse after tracer injection

This equation can be simplified into the form of a transfer function by the use of the backward shift operator z^{-1} which has the effect of replacing the c_{k-1} term by $z^{-1}.c_k$. The resulting expression is -

$$\frac{c_k}{u_{k-1}} = \frac{\phi}{1-(1-\phi)z^{-1}} \quad (2b)$$

Where ϕ is the ratio of pulse to system volume

(b) Zero-mixing. If the entering pulse simply displaces an equal volume of existing system fluid and subsequently retains its identity, without mixing with its surroundings, this process is described as follows:-

$$c_k = u_{k-\tau} \quad (3)$$

where τ is the delay-time between pulse entry and exit

The pulses are assumed to leave in the same order as they enter the system; in consequence the delay-time (i.e. residence-time) for each pulse is identically equal to τ. This mixing limit is analogous to the 'plug-flow' condition in continuous flow systems.

(c) Partial mixing. Intermediate degrees of mixing of the inlet pulse with its surroundings can be characterized by regarding the total flow system as a structure of sub-regions, each of which behaves as either a zero-mixed or completely-mixed entity. Figures 2a, 2b and 2c show examples of this process. Once the structure is formulated it is not a difficult matter to combine the transfer function models of each of the sub-regions into an overall transfer model for the whole system. This results in an input-output transfer function model with the general functional relationship -

$$\frac{c_k}{u_{k-\tau}} = \frac{B(z^{-1})}{A(z^{-1})} \quad (4)$$

where $A(z^{-1})$ and $B(z^{-1})$ are polynomials in the transfer function operator z^{-1}.

Estimation of transfer function model parameters

The practical problem of interest is the reverse of the process described above. From measurements of the input/output data we first need to infer the best estimates of the coefficients in the transfer function model equation (4); then the overall transfer function model is decomposed into sub-elements which can be associated with a sub-regional structure for the overall flow system. The parameter estimation method used in this paper is that developed by Young (1984) based on the instrumental variable method of analysis, details of which can be found in his book.

CASE STUDY

Experimental data

The data used in this study are taken from a paper by Thirumurthi (1969) on performance studies of a laboratory-scale waste stabilization pond. The pond was operated semicontinuously whereby a discrete amount of wastewater was added once a day and a corresponding amount of effluent displaced from the pond. The sequence of displaced effluent was monitored for organic content and the process was continued until steady-state was approached. The degree of removal of organic matter depended on the conditions of mixing in the pond as well as the kinetics of degradation and so a tracer experiment was carried out to determine the extent of mixing. A control pond of the same geometry as the experimental pond was filled with distilled water and a discrete volume of dilute sodium chloride solution added, equal to the feed volume of wastewater in the experimental pond. Thereafter the same volume of distilled water was added once a day and the displaced effluent monitored for sodium chloride. The results are shown as discrete points on Figure 3.

Determination of transfer function parameters

The measured sequence of input and output tracer concentrations over a period of 20 days was evaluated using a microcomputer package 'MICROCAPTAIN', developed by Young (1984) to implement the instrumental variable parameter estimation method referred to earlier. The user first has to nominate the orders of the polynomials $A(z^{-1})$ and $B(z^{-1})$ in the transfer function model described in equation (4), and the time-delay parameter. The 'MICROCAPTAIN' package then estimates the coefficients in the polynomials $A(z^{-1})$ and $B(z^{-1})$ and their standard errors; it also provides a coefficient of determination which is a normalised measure of how well the model explains the data, and an error variance norm which is a sensitive indicator of overparamerization. The user can therefore screen several transfer function models and choose the one giving the best compromise between the coefficient of determination and the number of parameters specified for estimation.

The transfer function model best describing the experimental results from Thirumurthi's study proved to be a second-order polynomial in $A(z^{-1})$, a third-order polynomial in $B(z^{-1})$ and a time-delay of 2 days. The coefficients in the polynomials are given below

$$A(z^{-1}) = 1 + a_1 z^{-1} + a_2 z^{-2} \quad (4a)$$

where $a_1 = -1.054$
$a_2 = 0.104$

$$B(z^{-1}) = b_o + b_1 z^{-1} + b_2 z^{-2} + b_3 z^{-3} \quad (4b)$$

where $b_o = 0.0038$
$b_1 = 0.0134$
$b_2 = 0.0208$
$b_3 = 0.0121$

The coefficient of determination was 0.999 indicating a very close explanation of the experimental results by the transfer function model. Figure 3 clearly shows the agreements between predicted and measured values.

Interpretation of the transfer function model

The second-order polynomial $A(z^{-1})$ can be factorized and the transfer function separated as a summation of sub-elements -

$$c_k = E_1.E_2.E_3$$

where $E_1 = \dfrac{0.056}{z^{-1} - 0.944}$

$$E_2 = \frac{0.890}{z^{-1} - 0.110}$$

$$E_3 = 0.076u_{k-2} + 0.268u_{k-3} + 0.415u_{k-4} + 0.242u_{k-5}$$

E_1, E_2 are elements representing completely mixed regions with mean-residence times of 17.9 and 1.1 days, respectively.

E_3 represents division of the fluid into parallel streams with delay times of 2, 3, 4 and 5 days, respectively.

The transfer function represents the flow of inlet fluid pulses through two completely-mixed regions in series followed by separation into parallel flow components with time-delays of 0, 1, 2, 3 days respectively, as shown in Figure 4. The relative proportion of the total system volume occupied by the various sub-regions is also shown in Figure 4. These values can be calculated from the mean residence-times spent by the inlet fluid in the sub-regions of the system; the mean residence-times for the completely-mixed regions are obtained from the sub-elements of the transfer function representing those regions while those for the zero-mixed regions are equal to their respective delay times.

DISCUSSION AND CONCLUSIONS

The transfer function model is shown to be a possible method of describing partial mixing in a semicontinuous flow system. As with analogous treatments of continuous flow systems, the approach of breaking down a total system into a series of linked sub-regions, each with its own zero-mixed or completely-mixed flow structure, has its limitations. Most critical is the lack, in most cases, of a direct correspondence between the proposed structure and the actual structure of the flow in the system. But the difficulty is that the physical processes of momentum and energy transfer responsible for the mixing in a system are usually too complex to analyse except in the simplest of cases, and so at this stage a less than desirable modelling approach must suffice. The models are nonetheless distinct advances on 'black-box' models where absolutely no reference is made to an internal structure of any kind, and their use in the design of continuous flow reactors, for example, is well proven. As a next step it is proposed to study the mixing produced by well-understood structures, such as vortex rings which could be produced with the semicontinuous feed injection process. In this way a link between the transfer function type of mixing model and the actual physical mixing mechanisms might be discerned.

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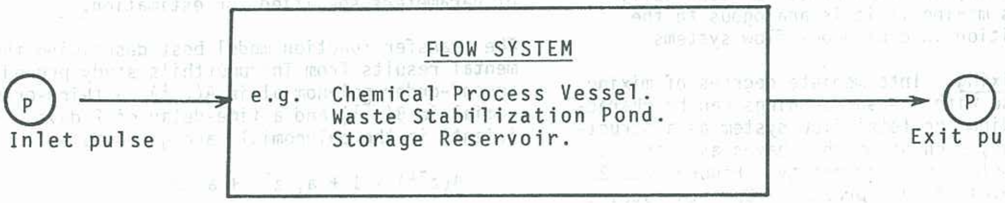


Fig. 1: Semicontinuous flow system: regular sequence of constant volume pulses fed to constant volume system with near-instantaneous injection

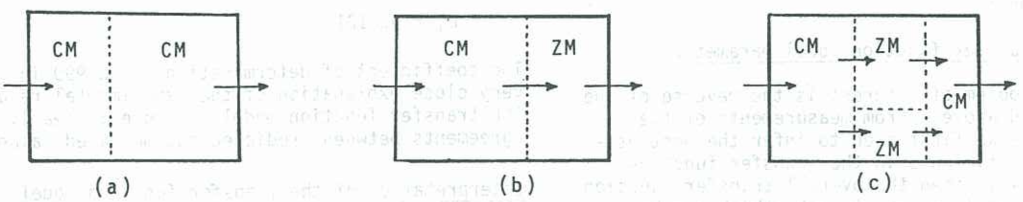
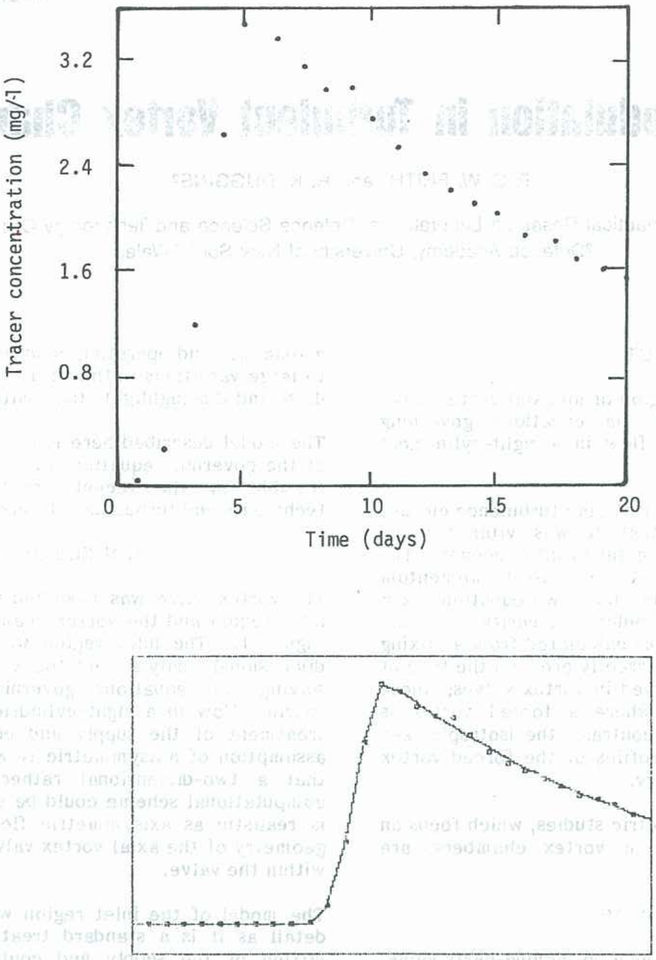
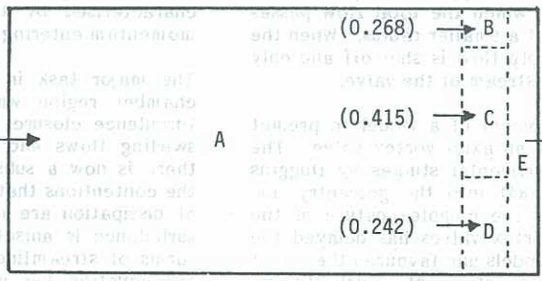


Fig. 2: Examples of division of system volume into a network of sub-regions of either complete-mixing (CM) or zero-mixing (ZM)



'MICROCAPTAIN' print-out showing the agreement between the experimental points and the proposed transfer function, Equations (4), (4a) and (4b)

Fig. 3 : Experimental tracer data Thirumurthi (1969) compared with predictions given by transfer function model.



Region A : CM occupying 85.5% of system volume
Region B : ZM occupying 1.3% of system volume
Region C : ZM occupying 4.3% of system volume
Region D : ZM occupying 3.5% of system volume
Region E : CM occupying 5.4% of system volume

Figures in parenthesis show relative pulse volumes. (note that a relative volume of 0.075 flows directly from Regions A to Region E and is not shown on the diagram).

Fig. 4 : Division of total system volume into sub-regions of either complete-mixing (CM) or zero-mixing (ZM).